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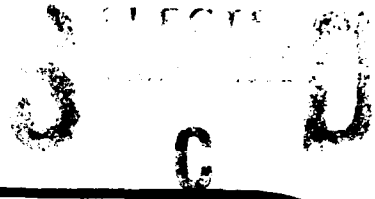

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CHEMICAL RESEARCH, DEVELOPMENT & ENGINEERING CENTER

CRDEC-TR-320

VAPOR PRESSURE OF n-AMYL ACETATE: LITERATURE REVIEW AND EXPERIMENTAL DETERMINATION

Ann Brozena
Helen M. Walker
Elwin C. Penski

RESEARCH DIRECTORATE

January 1992

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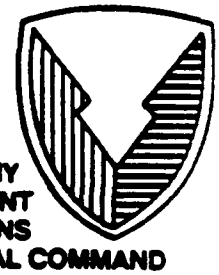

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13. ABSTRACT *(Maximum 200 words)*

A thorough review of literature vapor pressure data for n-amyl acetate revealed a conflict in values at ambient temperature. The vapor pressure of a pure sample of n-amyl acetate was determined directly by differential thermal analysis (DTA) and indirectly from evaporation rate. A best fit predictive equation describing vapor pressure of n-amyl acetate as a function of temperature has been generated which is more reliable than currently available literature data.

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PREFACE

The work described in this report was authorized under Project No. 1C162622A553L, CB Defense Assessment Technology. This work was started in April 1990 and completed in July 1991. The experimental data are recorded in laboratory notebooks 84-0195 and 85-0215.

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The authors wish to acknowledge Douglas R. Sommerville for providing the high purity sample of n-amyl acetate and Linda L. Szafraniec and William T. Beaudry for sample purity analysis by nuclear magnetic resonance spectroscopy. The technical advice of Donald Fielder and editorial comments of Vincent M. McHugh are also greatly appreciated.

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CONTENTS

LIST OF FIGURES

LIST OF TABLES

VAPOR PRESSURE OF n-AMYL ACETATE: LITERATURE REVIEW AND EXPERIMENTAL DETERMINATION

1. INTRODUCTION

N-amyl acetate is currently being used to evaluate a novel method [1] for determining droplet evaporation during free fall. This methodology is being employed in open air dissemination trials. Vapor pressure is one of the key physical properties required for validation of the method. A preliminary review [2] of numerous open literature sources of vapor pressure data revealed conflicting values at ambient temperature for n-amyl acetate.

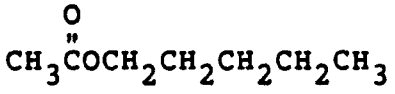
In an attempt to resolve this conflict, a thorough literature search and evaluation has been completed. Due to ambiguous nomenclature, poor documentation of sample purity, and the availability of only a limited amount of raw data, the literature vapor pressure data for n-amyl acetate have been judged to be inadequate for the current requirement.

The vapor pressure of n-amyl acetate of known purity has been determined directly by differential thermal analysis (DTA) and indirectly from its evaporation rate. A comparison of the experimental vapor pressure data with open literature values is presented.

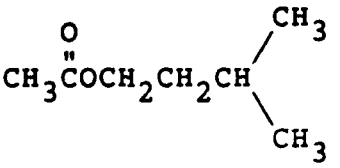
2. BACKGROUND

2.1 Nomenclature

Amyl acetate exists in several isomeric forms. The two most common isomers are shown below.



n-amyl acetate



iso-amyl acetate
(banana oil, pear oil)

The term "amyl acetate" is often used to refer to either isomer, with no distinction being made between the "normal" and "iso" forms, or a mixture of the two. Both materials are available commercially in several grades varying in composition and purity.[3] Citations of physical properties for either isomer rarely list sample purity even though some commercial grades can contain as little as 60% of the primary compound. This lack of unambiguous nomenclature and omission of sample purity in the open literature has resulted in confusion regarding the identity of the compound for which data are being reported.

2.2 Assessment of Literature Vapor Pressure Values

Routinely, assessment of literature vapor pressure information consists of locating raw experimental data from all available sources and evaluating it based on its agreement with other data, the experimental method used, and sample purity. Once the questionable data have been discarded, the remaining points are fit to an equation relating vapor pressure and temperature to permit calculation of vapor pressure at temperatures of interest. Numerous equations are available for expressing vapor pressure as a function of temperature; however, the Antoine equation [4] has been found to provide the best fit for routine application at CRDEC.

Locating all of the information required to objectively evaluate literature vapor pressure data is not a trivial matter. Determination of the vapor pressure of a compound and massaging the data into a useable form is a complicated process which can involve a wide variety of experimental methods and data analysis techniques. The details of this process are critical to accurately assessing experimental data; unfortunately, they are frequently omitted from literature citations. Published data appear in many forms ranging from the detailed account of experimental method with accompanying table of raw data to the shorthand, equation format with no reference to valid temperature range or source data. While it is recognized that space limitations often dictate how much information can be provided, the lack of even a reference to supporting documentation can render some sources useless to the data evaluator.

2.3 Evaluation of n-Amyl Acetate Vapor Pressure Literature

The search for vapor pressure data for n-amyl acetate consisted of checking common secondary sources (compilations, handbooks, and databases) and any primary source articles referenced therein, if available. A detailed listing and evaluation of the information located in each source is provided in Appendices A through G. The Appendices are arranged chronologically by secondary source. The nomenclature and molecular structure (if given) are listed for each source to illustrate the ambiguity in this area. If provided in the source document, sample purity is also listed. Where necessary, conversions to temperature in °C and pressure in Torr were made to allow easier comparison among different references.

A comparison of the vapor pressure at 25 °C and boiling point at 760 Torr from these sources is given in Table 1. Where a table of values rather than an equation was provided in the source document, an Antoine equation was generated and the value at 25 °C calculated for inclusion in this table.

Table 1. Comparison of Literature Vapor Pressure Values for n-Amyl Acetate

Source	Vapor Pressure at 25 °C (Torr)	Boiling Point* (°C)	Appendix Citation	Reference
Jordan	4.0	147	A	5
Davis	4.0	147	A-1	6
Gardner	-	-	A-1-1	7
Riddick/Toops	98.2**	149.2	B	8
Schmidt	9.6	137.9	B-1	9
Vogel	-	148***	B-2	10
Hannotte	-	148.8	B-3	11
Mumford et al.	-	149.2	B-4	12
Marsden/Mann	-	146	C	3
Dykyj/Repas	4.5	148.9	D	13
Davis	4.0	147	D-1	6
Gardner	-	-	D-1-1	7
Timmermans et al.	-	149.6	D-2	14
Usanovich et al.	11.8	-	D-3	15
DIPPR	3.5	149.4	E	16
TRC	9.7	149.4	E-1	17
Riddick et al.	6.0	149.2	E-2	18
Davis	4.0	147	E-2-1	6
Gardner	-	-	E-2-1-1	7
Vogel	-	148**	E-2-2	10
Hannotte	-	148.8	E-2-3	11
Mumford et al.	-	149.2	E-2-4	12
Reidel	-	-	E-3	19
CHRIS	5.4	149.2	F	20
Riddick/Bunger/Sakano	9.7	149.2	G	21
Davis	4.0	147	G-1	6
Gardner	-	-	G-1-1	7
TRC	9.7	149.4	G-2	17

* Boiling point at 760 torr unless otherwise noted.

** This is not a typographical error. This compilation misquoted the source reference and lists data for ethyl acetate instead of n-amyl acetate.

*** Boiling point at 762 torr.

A cursory review of the values, prior to any points being rejected, revealed reasonable agreement among the reported atmospheric pressure boiling points. However, a significant spread was noted in the values from 1 to 10 Torr, the pressure range of interest for the intended application of these data. This was not unexpected due to the difficulties associated with accurately determining vapor pressure in this range.

The specific reasons for acceptance or rejection of each source are listed with the evaluation in the Appendices. Table 2 contains a summary of these reasons. The criteria for acceptance or rejection of a citation was based primarily on how much information was provided. A citation was only as good as its raw source data since these were ultimately evaluated. Care had to be exercised to distinguish raw "data" from calculated "values" (data which had been fit to an equation). Smoothing can mask significant errors in raw data which can go undetected unless some measure of the fit is provided. Thus, smoothed values, even from compilations which did reference source data, were rejected.

The problems of ambiguous nomenclature and lack of sample purity information were frequently encountered among the literature citations. Though these did not constitute sufficient justification for deleting a set of values from further consideration, they did complicate the assessment process. In general, most secondary sources do not state sample purity and this was taken into account in the evaluation process. However, it is reasonable to expect the issue of purity to be addressed in primary source articles. Given what is known about the commercial grades of n-amyl acetate, it is possible that the spread in ambient vapor pressure values is due to variations in sample purity. This cannot be confirmed since only two of the sources stated sample purity and these have been rejected due to lack of reference to source data.

Several of the literature sources contained only atmospheric pressure boiling points which were determined during preparation of the sample for measurement of other properties. Evaluation of these sources was done with somewhat more leniency than articles whose specific intent was to measure vapor pressure of the compound. The absence of discussion of experimental method or sample purity for these sources did not result in their being rejected since the conflict in literature data centered around the low pressure range rather than values at atmospheric pressure.

With all of the objectionable values rejected, only three data sets remained (Schmidt, Gardner, and Usanovich, et. al.) Comparison of these sets still showed a significant spread which is illustrated in Figure 1. It was concluded that the conflict in literature vapor pressure data for n-amyl acetate could not be resolved and that additional measurements had to be made on a sample of known purity.

Table 2. Evaluation of Literature Vapor Pressure Values for n-Amyl Acetate

Source	Assessment	Reason
Jordan	accept	good source - cites Davis's Antoine equation and gives temperature range
Davis	accept	Antoine equation generated from Gardner's data
Gardner	accept	appears to contain good data but only plot is given - no data table
Riddick/Toops	reject	extracted data for wrong compound from source
Schmidt	accept	appears to be good data - misquoted by Riddick
Vogel	accept	boiling point only
Hannotte	accept	boiling point only
Mumford	accept	boiling point only
Marsden/Mann	reject	no source references given
Dykyj/Repas	reject	Clausius-Clapeyron equation listed not Antoine
Davis	accept	Antoine equation generated from Gardner's data
Gardner	accept	appears to contain good data but only plot is given - no data table
Timmermans	accept	boiling point only
Usanovic	accept	limited raw data - sample distilled
DIPPR	reject	majority of values presented are smoothed
TRC	reject	smoothed values
Riddick	accept	lists Davis's Antoine equation but gives incorrect value at 25°C
Davis	accept	Antoine equation generated from Gardner's data
Gardner	accept	appears to contain good data but only plot is given - no data table
Vogel	accept	boiling point only
Hannotte	accept	boiling point only
Mumford	accept	boiling point only
Reidel	reject	article contains derivation of equation - no data
CHRIS	reject	no source references given
Riddick/Bunger/ Sakano	reject	another fit of smoothed TRC values
Davis	accept	Antoine equation generated from Gardner's data
Gardner	accept	appears to contain good data but only plot is given - no data table
TRC	reject	smoothed values

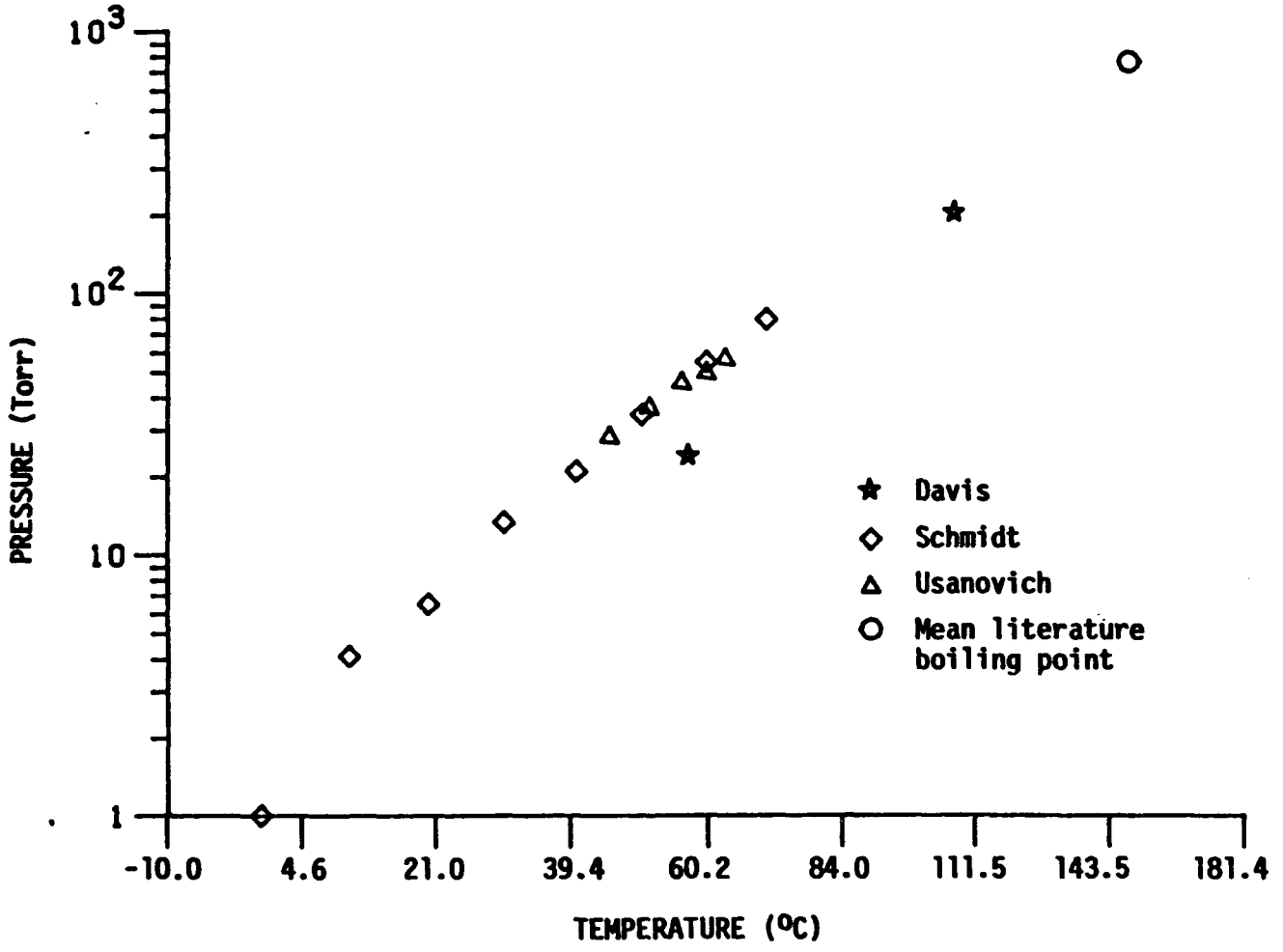


Figure 1. Literature Vapor Pressure of n-Amyl Acetate - Accepted Data Sets.

3. EXPERIMENTATION

3.1 Materials

The n-amyl acetate used in this work was obtained from EM Science, Cherry Hill, NJ. The sample was determined to be > 99 mole % pure by ^{13}C nuclear magnetic resonance (NMR) spectroscopy.

3.2 Methods

3.2.1 Vapor Pressure by Differential Thermal Analysis (DTA)

A DuPont Model 9900 Differential Thermal Analysis (DTA) System (DuPont Instruments Company, Wilmington, DE) was used to measure vapor pressure from 18 to 148 °C using the modified DTA method.[22,23,24] The accuracy reported for this method was ± 5%.

3.2.2 Droplet Evaporation Measurements

The evaporation of a suspended droplet of n-amyl acetate was measured by methodology previously described.[25]

4. RESULTS

4.1 DTA Data

The experimental DTA data were analyzed by the computer method developed by Penski and Latour [26] to derive the constants for the Antoine vapor pressure equation shown below:

$$\log_{10} P = A - B/(C+t) \qquad (1)$$

where

P = vapor pressure in Torr
t = temperature in °C
A, B, C = constants

The standard deviation of $\log_{10}P$ was calculated using the following equation:

$$SD = \left(\frac{S}{n-1} \right)^{1/2} \qquad (2)$$

where

n = number of points

$$S = \Sigma(\log P_{calc} - \log P_{exp})^2 \qquad (3)$$

The logarithmic values were used since it has been reported that this procedure prevents excess weighting of higher vapor pressure data.

The constants derived for the Antoine equations were then used to calculate the heats of vaporization in kcal/mole and the volatilities in g/m^3 at selected temperatures from the following respective equations:

$$\Delta H_{vaporization} = 2.303\ RB \left(\frac{T}{C+t} \right)^2 \qquad (4)$$

$$Volatility = \frac{PM}{760\ R'T} \qquad (5)$$

where B and C = Antoine equation constants

t = temperature in degrees centigrade

T = temperature in Kelvin

M = molecular weight in grams/mole

R = gas constant

= 1.987×10^{-3} kcal/mole K

R' = gas constant

= 82.05×10^{-6} atm m^3/mole K

Table 3 contains the experimental and calculated vapor pressure data for n-amyl acetate at the experimental temperatures. At the top of the table are the Antoine constants used to generate the calculated vapor pressures, the standard deviation of the Antoine equation, and the calculated boiling point for n-amyl acetate. This table also contains the percentage of difference between the experimental and calculated values. The calculated vapor pressure, volatility, and heat of vaporization for n-amyl acetate at selected temperatures are listed in Table 4. The starred (*) values in this table are extrapolated outside the experimental temperature range. Shown in Figure 2 is a plot of the experimental and calculated vapor pressure versus temperature (the symbols are experimental points and the line is the calculated vapor pressure from the Antoine equation).

4.2 Droplet Evaporation Data

The results of the droplet evaporation measurements are given in the first two columns of Table 5.

Assuming a vapor pressure of 2.6 Torr at 23 °C, the third and fourth columns were calculated in Table 5 using the model for a spherical droplet.[27]

Table 3. Experimental and Calculated Vapor Pressure of n-Amyl Acetate

Antoine Constants	
A	6.73665
B	1254.46
C	176.901
Standard Deviation of $\log_{10}P$	0.015
Calculated Boiling Point (°C)	148.44

Temperature (°C)	Vapor Pressure (Torr) Experimental	Calculated	Percent Difference
18.5	2.0	2.07	3.68
23.6	3.1	3.02	-2.57
30.7	5.0	4.94	-1.13
36.2	7.0	7.08	1.13
41.1	10.1	9.60	-4.95
48.3	15.0	14.66	-2.24
55.4	20.1	21.70	7.97
72.1	50.2	49.97	-0.46
87.7	100.0	99.02	-0.98
117.8	299.9	301.95	0.68
148.4	763.5	759.20	-0.56

Table 4. Calculated Properties of n-Amyl Acetate at Selected Temperatures

Temperature (°C)	Vapor Pressure (Torr)	Volatility (mg/m^3) ($x10^{-4}$)	Heat of Vaporization (kcal/mole)
0.0*	0.4419	0.3378	13.69
5.0*	0.6923	0.5196	13.42
10.0*	1.059	0.7805	13.17
15.0*	1.584	1.147	12.94
20.0	2.321	1.653	12.72
25.0	3.338	2.337	12.52
30.0	4.716	3.248	12.32
35.0	6.556	4.441	12.14
40.0	8.977	5.984	11.97
45.0	12.12	7.951	11.80
50.0	16.14	10.43	11.64
55.0	21.24	13.51	11.49
60.0	27.63	17.31	11.35
65.0	35.55	21.95	11.22
70.0	45.27	27.54	11.09
75.0	57.11	34.24	10.96
80.0	71.39	42.20	10.85
85.0	88.48	51.57	10.73
90.0	108.8	62.53	10.63
95.0	132.7	75.27	10.52
100.0	160.8	89.96	10.42

Table 4. Calculated Properties of n-Amyl Acetate at Selected Temperatures (continued)

Temperature (°C)	Vapor Pressure (Torr)	Volatility (mg/m^3) ($x10^{-4}$)	Heat of Vaporization (kcal/mole)
105.0	193.5	106.8	10.33
110.0	231.3	126.0	10.24
115.0	274.9	147.8	10.15
120.0	324.7	172.4	10.07
125.0	381.5	200.0	9.983
130.0	445.8	230.8	9.905
135.0	518.4	265.2	9.829
140.0	600.0	303.2	9.756
145.0	691.2	345.1	9.686
150.0	792.9	391.2	9.618

Table 5. Evaporation of a Suspended n-Amyl Acetate Droplet at 23 °C, 0.63 cm/s Nitrogen Atmosphere Velocity and Zero % Relative Humidity.

Time (hr)	Measured Mass (mg)	Calculated Mass (mg)	Diameter (mm)
0.0	2.71	2.71	1.78
0.018	2.48	2.57	1.76
0.051	2.30	2.32	1.72
0.101	1.96	1.96	1.62
0.151	1.62	1.62	1.52
0.251	0.98	1.02	1.31
0.331	0.51	0.61	1.10
0.501	0.03	0.04	0.87

The following equation was used to estimate the diffusion coefficient:

$$\text{Diffusion coefficient (cm/s)} = 1.82\ 10^{-4}\ M^{-0.5}\ T^{3/2} \qquad (6)$$

Where M = molecular weight
T = temperature in Kelvin

5. DISCUSSION

The vapor pressure data generated for n-amyl acetate, by both DTA and evaporation rate, show values lower than those given in the literature by Davis, Schmidt, and Usanovich. A

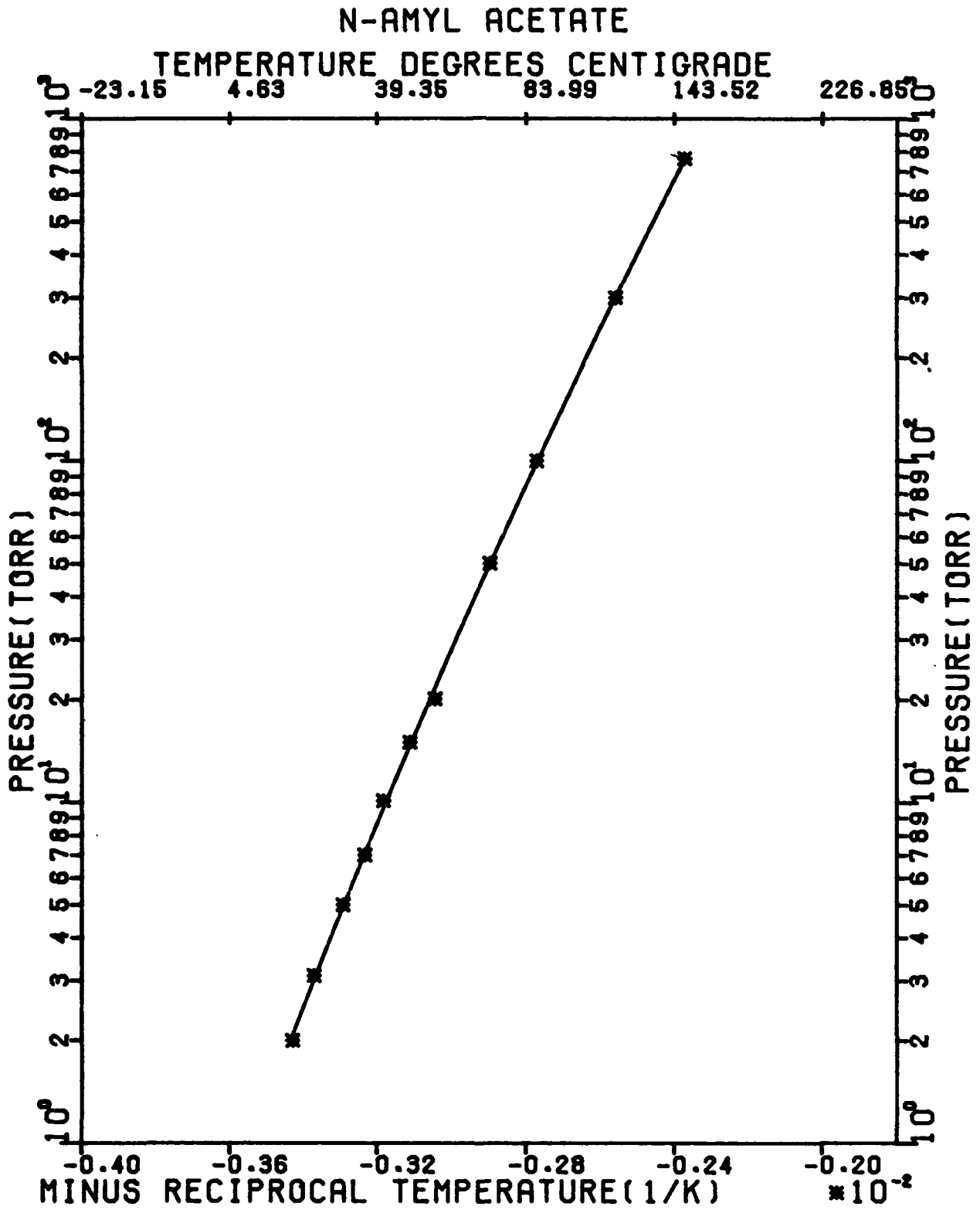


Figure 2. Vapor Pressure of n-Amyl Acetate by Differential Thermal Analysis.

comparison of these values at 23 °C (the temperature at which evaporation data was generated) is listed in Table 6. A plot of the experimental data and the values from Davis, Schmidt, and Usanovich is shown in Figure 3.

Table 6. Comparison of Experimental and Literature Vapor Pressure Values for n-Amyl Acetate

Source	Vapor Pressure at 23 °C (Torr)
DTA	2.9*
Evaporation	2.6
Schmidt	8.5*
Davis	3.6*
Usanovich	10.8*

*Calculated from Antoine equation.

The differences between the literature vapor pressure of n-amyl acetate and the data generated by DTA and evaporation rate are somewhat difficult to account for in the absence of sample purity information from the literature sources. Based on what is known about the availability of n-amyl acetate in various grades, it is assumed that the differences are due to variations in sample purity. The presence of low boiling impurities would explain the higher literature values. This would be consistent with the lower values generated by DTA and calculated from evaporation rate since the sample used for that work was known to be of high purity (> 99 mole %). As a result, the data generated in this work is considered to be more reliable than any of the values currently in the open literature. It is recommended that the values found in Tables 3 and 4 be used where accurate vapor pressure data for pure n-amyl acetate is required.

The slight difference between the DTA and evaporation data can be attributed to the method used to calculate vapor pressure from evaporation rate. The diffusion coefficient used in the calculation was not available for n-amyl acetate and thus had to be estimated. Inaccurate estimation of this value can result in as much as a 20% error in the calculated vapor pressure.

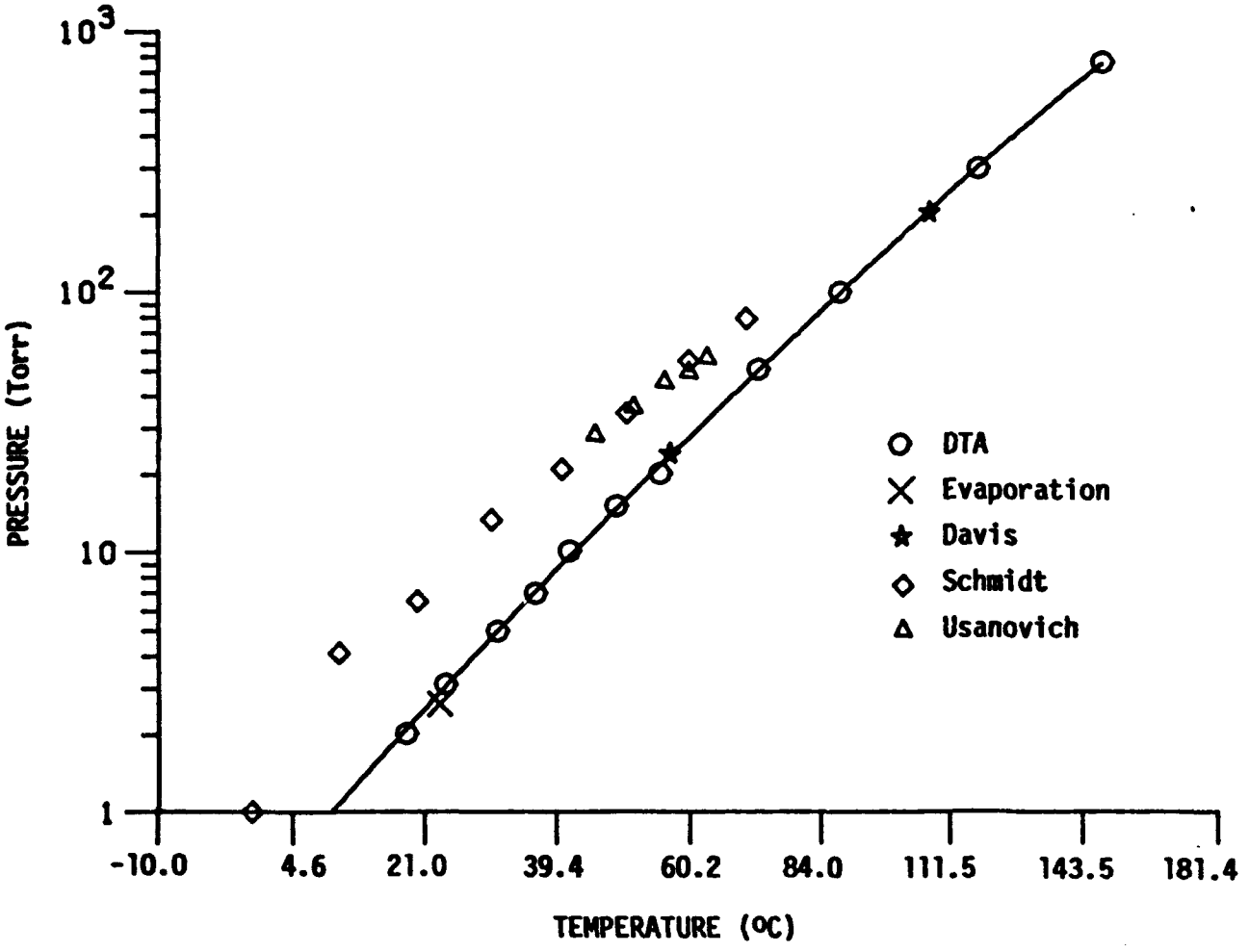


Figure 3. Experimental vs. Literature Vapor Pressure of n-Amyl Acetate.

6. CONCLUSION

- A thorough review of the literature vapor pressure citations for n-amyl acetate revealed a conflict in published values at ambient temperatures.

- The vapor pressure of n-amyl acetate has been determined over a wide temperature range using differential thermal analysis (DTA) and evaporation rate data.

- Table 3 provides the experimental and calculated DTA vapor pressure data at the experimental temperatures.

- Table 4 provides calculated vapor pressure, volatility, and heat of vaporization at selected temperatures.

- Table 5 provides the results of the droplet evaporation measurements.

- Constants for a best fit predictive Antoine equation expressing vapor pressure as a function of temperature are provided at the top of Table 3. This equation can be used to calculate vapor pressure to determine droplet evaporation during free fall.

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27. Penski, E.C., The Evaporation of Macroscopic Droplets, I. Theoretical Factors for a Two Component System, CRDEC-TR-88124, U.S. Army Chemical Research, Development and Engineering Center, Aberdeen Proving Ground, MD, June 1988, UNCLASSIFIED Report.

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APPENDIX A

SOURCE DOCUMENTS A

Secondary Source A

Jordan, E.T., "Vapor Pressure of Organic Compounds," Interscience Publishers, New York, 1954.

amyl acetate

$C_7H_{14}O_2$

Boiling point = 147 °C at 760 Torr

$$\log P = 8.078 - \frac{2077}{t + 253}$$

Range = 0 to 147 °C
t = temperature (°C)
P = pressure (Torr)

COMMENTS: The nomenclature in this source is ambiguous however, the Antoine equation listed is taken directly from a primary source which identifies the compound as n-amyl acetate. Also, this is one of only two sources which state a temperature range over which the listed vapor pressure equation is valid. This information is critical if errors due to extrapolation are to be avoided. This compilation is an acceptable source.

Primary Source A-1

Davis, D.S., "Line Coordinate Chart for Vapor Pressures of Organic Solvents," Ind. Eng. Chem., 33, 401, (1941).

n-amyl acetate

$$\log P = 8.078 - \frac{2077.3}{t + 253}$$

t = temperature (°C)
p = pressure mm Hg

Table A-1. Vapor Pressure of n-Amyl Acetate from Davis

Temperature (°C)	Pressure (Torr)
56.9	23.9
106.6	204

COMMENTS: This article presents a nomograph for calculating vapor pressure based on raw data provided by Gardner (see Source A-1-1 below) which Davis then fit to an Antoine equation. Gardner's data set, consisting of thirteen points, was provided to Davis in a private communication. Unfortunately, Davis published only two of the raw points to illustrate the accuracy of his nomograph. Though not strictly a primary source article, Davis provides more useful vapor pressure data than does Gardner which results in this source being judged acceptable.

Primary Source A-1-1

Gardner, G.S. "Evaporative Index," Ind. Eng. Chem., 32, 226, (1940).

n-amyl acetate

Thirteen raw data points are given on a small plot from which the coordinates of each point cannot be accurately extracted.

COMMENTS: This article discusses evaporation rate of selected liquids. Measurement of vapor pressure was incidental; it was only done where satisfactory results "do not exist in the literature". The sample was apparently of acceptable purity as indicated by a narrow boiling range (145-147 °C). Unfortunately, presentation of the experimental data only as a plot renders this article basically useless as a source of raw data. It was accepted as a source for this work due to Davis' use of the data.

APPENDIX B

SOURCE DOCUMENTS B

Secondary Source B

Riddick, J.A. and Toops, E.E., "Organic Solvents: Physical Properties and Methods of Purification," Second Ed., Interscience Publishers, New York, 1955.

amyl acetate

$CH_3COOCH_2(CH_2)_3CH_3$

Table B-1. Vapor Pressure of Amyl Acetate from Riddick and Toops

Temperature (°C)	Pressure (Torr)
0	27.2
20	76.5
30	124.9
50	287.6
70	603
149.2	760

COMMENTS: Inclusion of the structure in this article clarifies the ambiguity in nomenclature. Unfortunately, except for the boiling point, the data cited are for ethyl acetate rather than amyl acetate. The source article (Schmidt) presented data for both compounds in the same table. Riddick and Toops extracted values for the wrong compound. This compilation is rejected as a source.

Primary Source B-1

Schmidt, E.C., "Binare Gemische," Z. Physik. Chem., 121, 221, (1926).

amyl acetate

Table B-2. Vapor Pressure of Amyl Acetate from Schmidt

Temperature (°C)	Pressure (Torr)
0	1.0
10	4.1
20	6.5
30	13.3
40	20.8

Table B-2. Vapor Pressure of Amyl Acetate from Schmidt (continued)

Temperature (°C)	Pressure (Torr)
50	34.5
60	54.6
70	78.9

COMMENTS: This article presents vapor pressure data for selected binary mixtures of organic liquids. For each mixture, the vapor pressure of the pure components is also given. Experimental method is discussed as is the importance of sample purity however, no specific purity is given for any of the samples. The amyl acetate data is presented on a table with ethyl acetate data. This source is acceptable.

Primary Source B-2

Vogel, A.I., "Physical Properties and Chemical Constitution. Part XIII. Aliphatic Carboxylic Esters," J. Chem. Soc., 624, (1948).

n-amyl acetate

Boiling point: 147-148 °C at 762 Torr
(mainly 148 °C)

COMMENTS: This article contains parachors and refractivities of selected esters. The boiling point is provided with a description of the preparation of the sample. Though it contains only a limited amount of information, this article is acceptable.

Primary Source B-3

Hannotte, T.A., "Azeotropic Mixtures of the Formates and Acetates of the Saturated Aliphatic Alcohols," Bull. Soc. Chem. Belg., 35, 86, (1926).

amyl acetate

Boiling Point: 148.8 °C at 760 Torr

COMMENTS: This article contains property data on selected azeotropic mixtures. It is acceptable.

Primary Source B-4

Mumford, S.A. and Phillips, J.W.C., "The Physical

Properties of Some Aliphatic Compounds," J. Chem. Soc., 75 (1950).

n-amyl acetate

Boiling point: 149.2 °C at 760 Torr

COMMENTS: This article contains selected physical property data generated for calculation of parachor. It is acceptable.

Appendix B

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APPENDIX C

SOURCE DOCUMENTS C

Secondary Source C

Marsden C. and Mann, S., "Solvents Guide," Interscience Publishers, New York, 1963.

primary amyl acetate

$CH_3COOC_5H_{11}$

60% n-amyl acetate
35% 2-methylbutyl acetate
5% 3-methylbutyl acetate

Boiling Point:
at 760 Torr: 146 °C
at 50 Torr: 50 °C
at 10 Torr: 10 °C

Vapor Pressure at 20 °C: 3.8 Torr

COMMENTS: Though this compilation uses clear nomenclature and lists compound purity, the lack of reference to any source for the cited value makes it unacceptable.

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APPENDIX D

SOURCE DOCUMENTS D

Secondary Source D

Dykyj, J. and Repas, M., "Tlak Nasytenej Pary Organiskych Zlucenin," Vydavatelstvo Slovenskey Akademie Vied, Bratislava, Czechoslovakia, Vol. I, 1979.

pentylacetat

$C_7H_{14}O_2$

$$\log P = 7.3560 - \frac{2258.3}{t + 273.15}$$

t = temperature (°C)
p = pressure (kPa)
range = 56 to 150 °C

Table D-1. Vapor Pressure of "Pentylacetat" from Dykyj and Repas

Temperature (°C)	Pressure (kPa)	(Torr)
39	1.333	10
53	2.666	20
67.5	5.333	40
76.8	7.999	60
89.3	13.332	100
107.7	26.664	200
128.0	53.329	400
148.9	101.325	760
159	133.322	1000

COMMENTS: Though the nomenclature and structure used to identify the compound are somewhat ambiguous, this compilation also lists a separate entry for "izopentylacetat", indicating that "pentylacetat" refers to n-amyl acetate. Davis (see source A-1) is cited as a source however his Antoine equation is not given. Instead, a Clausius-Clapeyron equation, presumably another fit of values calculated from Davis' Antoine equation, is presented which results in this source being rejected.

Primary Source D-1

Davis, D.S., "Line Coordinate Chart for Vapor Pressures of Organic Solvents," Ind. Eng. Chem., 33, 401, (1941).

[See source A-1]

Primary Source D-1-1

Gardner, G.S. "Evaporative Index," Ind. Eng. Chem., 32, 226, (1940).

[See source A-1-1]

Primary Source D-2:

Timmermans, J. and Hennaut-Roland, "Travaux Du Bureau International D'Etalons Physico-Chimiques: IX. Etude des Constantes physiques de vingt composes organiques," J. Chim. Physique, 52, 223, (1955).

n-amyl acetate

Boiling Point: 149.55 °C at 760 Torr

COMMENTS: This article contains selected physical properties for a variety of solvents and is an acceptable source

Primary Source D-3:

Usanovich, M., Bilyalov, K., and Krasnomolova, L., "Oxonium Compounds of Esters with Organic Acids," Z. Obsc. Chim., 25, 471, (1955).

amyl acetate

$CH_3COOC_5H_{11}$

Table D-2. Vapor Pressure of Amyl Acetate from Usanovich, Bilyalov, & Krasnomolova

Temperature (°C)	Pressure (Torr)
45	28
51	36
56	45
60	49
63	56

COMMENTS: Both nomenclature and structure given in this source are ambiguous. Purity is not provided though samples were subjected to repeated fractional distillation. Experimental method is discussed and is adequate. This source is acceptable.

APPENDIX E

SOURCE DOCUMENTS E

Secondary Source E

The Design Institute for Physical Property Data (DIPPR) Database. Project of the American Institute of Chemical Engineers. Pennsylvania State University.

n-pentyl acetate, banana oil, pear oil, primary amylacetate, 1-pentyl acetate

$CH_3COOCH_2(CH_2)_3CH_3$

Table E-1. Vapor Pressure of n-Pentyl Acetate from DIPPR

Temperature (K)	Temperature (°C)	Pressure (Pa)	Pressure (Torr)	Source
299.15	26	1.3332E+03	10	E-1
312.15	39	2.6664E+03	20	
321.15	48	3.9997E+03	30	
327.15	54	5.3329E+03	40	
333.15	60	6.6661E+03	50	
345.15	72	1.0666E+04	80	
351.15	78	1.3332E+04	100	
363.15	90	1.9998E+04	150	
372.15	99	2.6664E+04	200	
386.15	113	3.9997E+04	300	
396.15	123	5.3329E+04	400	
405.15	132	6.6661E+04	500	
412.15	139	7.9993E+04	600	
421.15	148	9.8658E+04	740	
422.15	149	1.0132E+05	760	
425.15	152	1.0666E+05	800	
430.15	157	1.1999E+05	900	
298.15	25	7.9993E+02	6	E-2
202.35	-71	2.3610E-02	1.77E-04	E-3*
222.13	-51	4.0670E-01	3.05E-03	
241.92	-31	4.1650E+00	3.12E-02	
261.70	-12	2.8670E+01	2.15E-01	
281.48	8	1.4460E+02	1.08E+00	
301.26	28	5.7040E+02	4.28E+00	
321.05	48	1.8450E+03	1.38E+01	
340.83	68	5.0760E+03	3.81E+01	
360.61	89	1.2220E+04	9.17E+01	
380.39	107	2.6360E+04	1.98E+02	
400.18	127	5.1810E+04	3.89E+02	
419.96	147	9.4200E+04	7.07E+02	
439.74	167	1.6040E+05	1.20E+03	
459.52	186	2.5840E+05	1.94E+03	

Table E-1. Vapor Pressure of n-Pentyl Acetate from DIPPR (continued)

Temperature (K)	Temperature (°C)	Pressure (Pa)	Pressure (Torr)	Source
479.31	206	3.9720E+05	2.98E+03	
499.09	226	5.8680E+05	4.40E+03	
518.87	246	8.3880E+05	6.29E+03	
538.65	266	1.1670E+06	8.75E+03	
558.43	285	1.5870E+06	1.19E+04	
578.22	305	2.1220E+06	1.59E+04	
598.00	325	2.8000E+06	2.10E+04	

* Estimated by Riedel's method [see Source C-3].

[The following is Reidel's equation generated by DIPPR.]

$$\ln P = 75.753 - \frac{8051.2}{T} - [(7.4786)(\ln T)] + [(8.0921 \times 10^{-18})(T^6)]$$

T = temperature (K)
P = pressure (Pa)

Data from literature plus data predicted by Riedel's method used in regression.

COMMENTS: This compilation contains information of little or no use. The values listed are either smoothed, miscalculated, or referenced to no source. This, in combination with contradictory nomenclature, results in this source being rejected.

Primary Source E-1

Thermodynamics Research Center (TRC), "Selected Values of Properties of Chemical Compounds," Data Project, Texas A&M University, College Station, Texas (loose-leaf data sheets, extant, 1980).

COMMENTS: Values attributed to this source are calculated. TRC, like DIPPR, compiles literature data and has not determined the vapor pressure of n-amyl acetate experimentally. The values are an example of what Penski [2] refers to as "fits of numbers generated by fits". This source is rejected.

Primary Source E-2

Riddick, J.A., Bunger, W.B., "Organic Solvents: Physical Properties and Methods of Purification," Third Ed., Wiley-Interscience, New York, 1970.

$$\log P = 8.078 - \frac{2077}{t + 253}$$

t = temperature (°C)
P = pressure (Torr)

Vapor Pressure: 6 Torr at 25°C

COMMENTS: This source is acceptable but must be used with caution. The Antoine equation listed is the original generated by Davis (see source A-1) however, the value given at 25 °C is incorrect (should be 4 Torr at 25 °C).

Primary Source E-2-1

Davis, D.S., "Line Coordinate Chart for Vapor Pressures of Organic Solvents," Ind. Eng. Chem., 33, 401, (1941).

[See source A-1]

Primary Source E-2-2

Vogel, A.I., "Physical Properties and Chemical Constitution. Part XIII. Aliphatic Carboxylic Esters," J. Chem. Soc., 624, (1948).

[See source B-2]

Primary Source E-2-3

Hannote, T.A., "Azeotropic Mixtures of the Formates and Acetates of the Saturated Aliphatic Alcohols," Bull. Soc. Chem. Belg., 35, 86, (1926).

[See source B-3]

Primary Source E-2-4

Mumford, S.A. and Phillips, J.W.C., "The Physical Properties of Some Aliphatic Compounds," J. Chem. Soc., 75, (1950).

[See source B-4]

Primary Source E-3

Riedel, L., "Eine Neue Universelle Damfdruck-formal," Chem. Ing. Tech., 26, 83, (1954).

COMMENTS: This article describes derivation of Reidel's equation for expressing vapor pressure as a function of temperature. It contains no data and is rejected.

APPENDIX F

SOURCE DOCUMENTS F

Secondary Source F

Chemical Hazard Response Information System (CHRIS) Manual, Volume II, U.S. Department of Transportation, United States Coast Guard, 1984.

amyl acetate

85-96% (technical, commercial grade)

Table F-1. Vapor Pressure of Amyl Acetate from CHRIS

Temperature (°F)	Temperature (°C)	Pressure (PSI)	Pressure (Torr)
40	4.4	0.030	1.55
50	10.0	0.042	2.17
60	15.6	0.060	3.10
70	21.1	0.084	4.34
80	26.7	0.116	6.00
90	32.2	0.158	8.17
100	37.8	0.212	10.96
110	43.3	0.283	14.64
120	48.9	0.375	19.39
130	54.4	0.490	25.34
140	60.0	0.636	32.89
150	65.6	0.818	42.30
160	71.1	1.043	53.94
170	76.7	1.321	68.32
180	82.2	1.660	85.85
190	87.8	2.071	107.10
200	93.3	2.567	132.75
210	98.9	3.161	163.47
220	104.4	3.869	200.08
230	110.0	4.708	243.47
240	115.6	5.697	294.62
250	121.1	6.857	354.61
260	126.7	8.210	424.58
270	132.2	9.782	505.88
280	137.8	11.600	599.89
290	146.0	13.690	760.00

COMMENTS: This compilation contains property and hazard information to be used in response to emergencies occurring during transport of commercial chemicals on the waterways. For this purpose, this source is quite adequate. However, as a source of raw data on pure n-amyl acetate, this compilation is rejected due to lack of references.

BLANK

APPENDIX G

SOURCE DOCUMENTS G

Secondary Source G

Riddick, J.A., Bunger, W.B., and Sakano, T.K., "Organic Solvents: Physical Properties and Methods of Purification," Fourth Ed., John Wiley & Sons, New York, 1986.

pentyl acetate

$CH_3COOCH_2(CH_2)_3CH_3$

Vapor Pressure = 9.70 Torr at 25 °C

$$\log P = 6.3066 - \frac{1197}{t + 200}$$

t = temperature (°C)
P = pressure (Torr)

COMMENTS: This compilation references one acceptable source (Davis) and one which was rejected (TRC). Unfortunately, instead of publishing Davis' Antoine equation, TRC's calculated values were refit to another Antoine equation. As a result, this source is rejected.

Primary Source G-1

Davis, D.S., "Line Coordinate Chart for Vapor Pressures of Organic Solvents," Ind. Eng. Chem., 33, 401, (1941).

[See source A-1]

Primary Source G-2

Thermodynamics Research Center Data Project (formerly Manufacturing Chemists Association Research Project), Thermodynamics Research Center, College Station, Texas A&M University.

[See source E-1]

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DATE: 3-92

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SUPPLEMENTARY

INFORMATION

DEPARTMENT OF THE ARMY
U.S. Army Chemical Research, Development and Engineering Center
Aberdeen Proving Ground, Maryland 21010-5423

ERRATUM SHEET

11 June 1992

REPORT NO.	CRDEC-TR-320
TITLE	VAPOR PRESSURE OF n-AMYL ACETATE: LITERATURE REVIEW AND EXPERIMENTAL DETERMINATION
AUTHORS	Ann Brozena, Helen M. Walker, Elwin C. Penski
DATE	January 1992
CLASSIFICATION	UNCLASSIFIED

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Joseph J. Vervier
Director, Research Directorate

CRRATA HD-A234138

PREFACE

The work described in this report was authorized under Project No. 1C162622A553L, CB Defense Assessment Technology. This work was started in April 1990 and completed in July 1991. The experimental data are recorded in laboratory notebooks 84-0195 and 85-0215.

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This report has been approved for release to the public.

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